

Message

From: Strynar, Mark [/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=5A9910D5B38E471497BD875FD329A20A-STRYNAR, MARK]
Sent: 4/6/2017 12:51:47 PM
To: Detlef Knappe [knappe@ncsu.edu]
CC: Lindstrom, Andrew [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=04bf7cf26aa44ce29763fbc1c1b2338e-Lindstrom, Andrew]
Subject: RE: PFECA structures
Attachments: GenX series potential structures MJS 4-6-17.pptx

Detlef,

Here are the structures I have found using Chemspider and EPA Chemistry dashboard for the C3 through C7 (based on formulas) perfluoro ethers in the GenX series. I tried to include ONLY the reasonable ones for LC-ESI- mode.

Mark

From: Detlef Knappe [mailto:knappe@ncsu.edu]
Sent: Tuesday, April 04, 2017 8:35 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Subject: RE: PFECA structures

Thank you, Mark. Can you let me know whether there are other structures that might not be right in figure S5?
Detlef

On Apr 4, 2017 12:20 PM, "Strynar, Mark" <Strynar.Mark@epa.gov> wrote:

Detlef,

In figure S5 I think the structure is not correct from the 2015 SI. These were the suspected structures and we did not QTOFMS data at the time. If these were both correct we could tell them apart with MS/MS as they would likely cleave at the ether oxygen. The top would give a C2F5O (135) transition and the bottom a C3F7O (153) transition for the daughter assuming the O migrates with the fragment. If not we would get a C2F5 (119) and a C3F7 (169) transition respectively.

I think they are both GenX and the lower structure is correct.

Mark

From: Detlef Knappe [mailto:knappe@ncsu.edu]

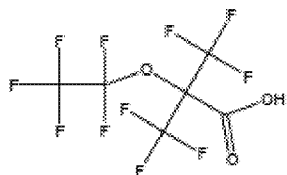
Sent: Tuesday, April 04, 2017 3:03 PM

To: Strynar, Mark <Strynar.Mark@epa.gov>

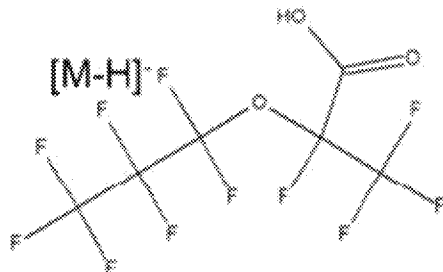
Subject: PFECA structures

Mark,

I am struggling with PFECA structures. In your 2015 paper, your homologous series (Figure S5) shows



Can we distinguish the above compound from GenX, which looks like this (same overall formula)



Detlef

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